Journal of Physics: Conference Series **388** (2012) 052079 doi:10.1088/1742-6596/388/5/052079

Electron and Positron Scattering from Pyrimidine

P. D. Palihawadana[*1], J. R. Machacek[*], C. Makochekanwa[*], J. P. Sullivan[*], M. J. Brunger[§], C. Winstead[†], V. McKoy[†], G. Garcia[$], F. Blanco[#], and S. J. Buckman[*]

[*] ARC Centre for Antimatter-Matter Studies, RSPE, The Australian National University, Canberra, Australia
[§] ARC Centre for Antimatter-Matter Studies, SCPES, Flinders University, Adelaide, Australia
[†] A. A. Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, CA, USA
[$] Instituto de Matemáticas y Física Fundamental, CSIS, Madrid, Spain
[#] Departamento de Física Atómica, Molecular y Nuclear, Universidad Complutense de Madrid, Madrid, Spain

Synopsis In this presentation we report the first low-energy measurements of elastic differential cross sections (DCS) for scattering of electrons (3-50 eV) by pyrimidine, along with cross sections calculated using the Schwinger multichannel variational technique (SMC), and a screening-corrected form of the independent-atom method, or the additivity rule, (SCAR). We also present total scattering, positronium formation, and differential cross sections recently measured at the positron beamline facility at the Australian National University, for positron (1-200 eV) scattering from pyrimidine.

The last decade has seen an enormous interest in the mechanisms of low-energy electron interactions with biologically relevant molecules. This has been driven by the recognition that those interactions can play a major role in biological processes, including DNA damage [1]. Studies in this field have extended from relatively simple, biologically relevant molecules such as water, to complex molecular constituents of DNA, and DNA itself. Obtaining absolute experimental reaction rates for processes such as dissociative attachment is notoriously challenging and it is hence important to benchmark state-of-the-art theory against experimental results for other scattering processes such as elastic scattering, excitation, and ionization.

Pyrimidine ($C_4H_4N_2$) is a model molecule for studying both electron and positron interactions with DNA/RNA bases, as three of the five nucleobases (cytosine, thymine, and uracil) are pyrimidine derivatives. But there are very few or no previous studies to be found in the literature on low energy electron and positron scattering from pyrimidine.

In figure 1, the present DCS measurements for 15 eV electron scattering are shown together with cross sections calculated using the SMC and SCAR methods. Here, the SCAR_n is obtained by normalizing the SCAR calculation in order to satisfy the optical theorem whereas the SCAR_n_d is derived by adding the dipole rotational excitation, calculated with the Born approximation. The present experimental DCS are in good qualitative agreement with the SMC results for all energies. However there are some differences in magnitude which exist between the two at intermediate angles, which could be due to the effect of neglecting open inelastic channels and hence over estimating the low-energy elastics cross section in the SMC calculation.

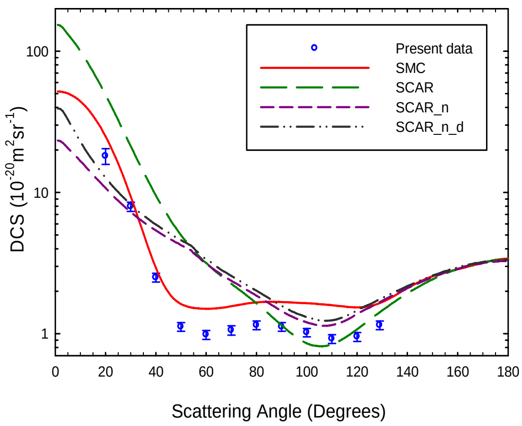

Figure 1. Present pyrimidine electron impact 15 eV DCS measurements with theoretical results.

The first DCS measurements for positron scattering from pyrimidine with other absolute cross sections, recently measured at the positron beamline facility at the Australian National University, will also be presented at the conference. These measured cross sections are used to discuss similarities and differences between electron and positron scattering processes.

This work was supported by the Australian Research Council. The work of CW and VM was supported by the US-DOE and the JPL.

References

[1] B Boudaiffa *et al.* 2000 *Science* **287** 1658

[1] E-mail: prp107@physics.anu.edu.au